REMARKS

Reconsideration of this patent application is respectfully requested in view of the foregoing amendments, and the following remarks.

Election/Restrictions

Election of invention

The Patent Examiner on Page 2 of the Office Action, has required the selection of one of the following inventions for the prosecution.

Group I. Claims 17, 3, 5-10, drawn to a Method of Making a Catalyst, classified in class 502, subclass 152.

Group II. Claim 4, drawn to Stochastic Fortran Algorithm as Random Check Generator, classified in class 341, subclass 109.

Group Ill. Claims 11-15, drawn to a Method of Using Catalyst in Multiple Catalytic Reactors, classified in 526, subclass 62.

The applicant respectfully selects with traverse Group I, as set forth in Claims 17, 3, 5-10 drawn to a Method of Making a Catalyst.

Election of species

The Patent Examiner on Page 3 of the Office Action, has stated that the application contains claims directed to more than one species of the generic invention.

The species are:

Active catalyst, selective catalyst, inorganic catalyst, organometallic catalyst, solid catalyst and non-solid catalyst.

Within the species, there is a sub species for solid catalysts as follows:

Chemical composition, weight composition, and catalyst properties.

Applicant is required to select a single species and if solid catalyst is chosen to select the sub species to which the claims shall be restricted to, even though this requirement is traversed.

The Applicant elects the single solid catalyst species with sub species chemical properties $V_{0.19}Mn_{0.24}Fe_{0.32}\ Ga_{0.25}\ O_x$ having a propane conversion of 22.3 %, a propene selectivity of 35.9 %, and a propene yield of 8.0 % (see table 8 Cat. No 4/74), with traverse. Newly added claim 18 is directed to this catalyst

species.

Traverse

The Applicant traverses the Requirement for Restriction for the following reasons:

Inventions I and III are not unrelated. The present application is drawn to a method of directed optimization of catalysts (page 4, lines 9-10). A person reasonably skilled in the art of optimization theory and catalyst design knows that an optimization procedure requires the following:

- the choice of an optimization method;
- a definition of an object to be optimized;
- a definition of how to optimize the object, the optimization step;
- a definition of a fitness or cost function in order to decide whether an optimization step leads to an improvement.

The optimization method of the present application is a genetic algorithm. The object to be optimized is a catalyst. The object is optimized by variation of the catalysts chemical and/or weight compositions. The fitness function of the present invention is defined by the catalysts properties, in particular

by their activity or selectivity or activity and selectivity of steps (b), (e), (h) and (k) of claim 17. The properties of each generations catalysts are determined experimentally in a reactor or in several connected reactors.

In contrast, *US Patent No. 6,763,309* of *Kieken et al.* determines the properties theoretically via machine learning methods, computation chemistry and micro-kinetic modeling (*US 6,763,309*, abstract). However, theoretical models are not as accurate as experimental determination and in addition are not as flexible. Any theoretical model needs to be adapted to the specific catalyst under investigation.

The optimization of catalysts requires the investigation of a very large number of different catalysts. It is therefore advantageous to use experimental determination of key catalysts properties. Still, the determination needs to be fast and efficient to provide an applicable optimization process. Claims 11-15 are drawn to the determination of the fitness function. They are inseparable linked and related to the method of claim 17.

Further, claims 11-15 are not independent claims, but are claims dependent upon claim 17. Also, the content of claims 11-15

is not a separate invention; but this is the best mode of determination of the fitness function for the selection of improved catalysts.

Also, inventions I and II are not unrelated. The optimization method of the present application is a Genetic Algorithm. A Genetic Algorithm requires the use of random numbers for selection, for the variation of the catalysts chemical and weight compositions. In respect, claim 17 refers to "randomly newly structuring" and claim 4 to one method for such randomly structuring. Further, claim 4 is not an independent claim, but a claim dependent upon claim 17. It does not contain a separate invention.

Furthermore, the Applicant traverses the requirement for election of a single disclosed species. The claims are drawn to a general method for selecting components for the preparation of [...] catalysts (Page 5, lines 24-26). They are not drawn to specific catalysts. This is supported by the examples which relate to different examples of material compositions and reactions.

It is respectfully pointed out that the documents cited by the Office Action, e.g. *US Patent No. 6,640,191* to *Deem et al.* on

combinatorial libraries related to the present invention are also not drawn to a specific catalyst while still being subjected to a search.

It is pointed out that both the corresponding PCT application and the corresponding European application have been classified in a class which comprises general catalytic processes. The aim of the present claims clearly is to develop a universally applicable strategy in the field of heterogenic catalysis, and to select effective catalysts from among a huge number of possible combinations. This aim is achieved by following the directed optimization as specified in claim 17.

In addition, it is believed that the present invention is directed to a unitary inventive concept, namely a method for selecting components of catalysts. Thus, it is believed that any search would necessarily include a search for the invention embodied in Group II and in Group III. Thus, a simultaneous search for all of the Groups is believed not to constitute an unreasonable search for the Patent Examiner. In addition, it is believed that the objectives of streamlined examination and compact prosecution would be promoted if a search were conducted simultaneously for all of the Groups. Also, the necessity of filing multiple patent applications for the same invention does

not serve to promote the public interest.

Applicant expressly reserves the right to file a divisional patent application for the non-selected inventions and for the non-elected species.

For all these reasons, it is respectfully requested that the requirement for restriction be withdrawn. An action on the merits of all the claims is respectfully requested.

Claim Objections

Claim 17 has been amended to recite "Periodic Table of Elements" and to cancel "PTE".

Claim Rejections - 35 USC § 112

The Patent Examiner on Page 5 of the Office Action, has stated that claims 17 and 3 to 15 are rejected under 35 U.S.C. 112, first paragraph, as failing to comply with the enablement requirement.

1. Method for preparing

The Patent Examiner has stated that the claims are drawn to "a method for preparing" yet as written seem to be a "method for selecting".

Based upon this comment in the Office Action, Claim 17 has been amended in the preamble to recite the following:

"Claim 17 A method for selecting components for the preparation of active and/or selective solid catalysts [...]"

The amendment is disclosed on page 5, lines 24-26, of the present application.

It is respectfully requested that the claim rejections regarding the enablement requirement related to "method for preparing" be withdrawn.

2. Arbitrarily or randomly

The Patent Examiner on page 6 of the Office Action has stated that claim 17 gives a method of "arbitrarily or randomly" preparing catalysts.

Claim 17 as amended is drawn to a method of "arbitrarily or randomly" selecting components of catalysts. It is known in the state of the art of optimization theory that random processes can be employed in an optimization step while still ensuring a directed optimization through use of a fitness or cost function.

For instance, *US Patent No. 6,640,191* to *Deem et al.* discloses the use of a Monte Carlo method for library design in computation chemistry. It is know in the art that a Monte Carlo method employs random numbers.

Petasis (US Patent NO. 6,602,817) discloses a combinational approach to chiral reagents or catalysts having amine or amino alcohol ligands. The Patent Examiner himself states on page 11, last paragraph, of the Office Action that "it is known in the art that the field of combinatorial chemistry requires random combination of chemicals [...]".

In the present application the optimization method is a Genetic Algorithm with a fitness function related to the properties of the selected catalysts. The Genetic Algorithm selects the components of catalysts randomly. However, it is also possible to employ prior knowledge of the person skilled in the art, e.g. in choosing the components for a first generation of a

catalysts, in one step, and then to continue the optimization by random selection.

Therefore, it is respectfully requested that the claim rejections regarding the enablement requirement related to the phrase "arbitrarily or randomly" be withdrawn.

3. Crossing and mutation

The Patent Examiner on page 7 of the Office Action has stated that the terms "crossing" and "mutation" are not functional connotations.

The Patent Examiner agrees that the present application defines the terms "crossing" and "mutation" on pages 9-10 of the specification.

However, it is stated in the Office Action that the term "crossing" in claim 17 is used by the claim to mean "exchanging", while the accepted meaning is "(genetics) the act of mixing different species or varieties of animals or plants and thus to produce hybrids". Furthermore, the term "mutation" in claim 17 is used by the claim to mean "reduce or enlarge", while the accepted meaning is "a relatively permanent change in hereditary material

involving either physical change in chromosome relations or a biochemical change in the codons that make up genes".

It is pointed out that the cited accepted meaning is related to the field of genetics. While it is true that the terms originate from the field of genetics, it is well known in the art of optimization theory and genetic algorithms that the terms can be transferred to abstract optimization problems. Applications are being discussed in the seminal books *"Adaptation in Natural and Artificial Systems: An Introductory Analysis with Applications to Biology, Control, and Artificial Intelligence" by John H. Holland (MIT Press, 1975)*, and *"Genetic Algorithms in Search, Optimization, and Machine Learning" by David E. Goldberg (Addison-Wesley, 1989)*. The back cover of the book by *Goldberg* reads:

> *"programmers, scientists, engineers, mathematicians, statisticians and management scientists will all find interesting possibilities here." (Goldberg, Genetic Algorithms in Search, Optimization, and Machine Learning, Addisson-Wesley)*

However, while the terms are generally transferable to abstract optimization problems,

"there is no single standard method by which a genetic algorithm generates a new population from the previous one[...]. Methods are usually problem-specific [...]." (Sheridan and Kearsley, J. Chem. Inf. Comput. Sci. 1995, 35, 310-320, p. 313, fourth paragraph).

The present application redefines the terms "crossing" and "mutation" on page 9-10 of the specification and specifies them in steps (d), (g) and (j) of claim 17. Steps (d), (g) and (j) specify that the catalysts components are exchanged (crossing) or that the substance amounts are varied (mutation), or that exchange (crossing) and variation (mutation) are performed.

Claim 17 has been amended to specify the above mentioned terms further:

"[...] by means of crossing and mutation of steps (d), (g) and (j)" (Claim 17, present application).

It is respectfully requested that the claim rejections regarding the enablement requirement related to the terms "crossing" and "mutation" be withdrawn.

4. Random check generators, throwing dice and/or performing drawings

The Patent Examiner on page 8 of the Office Action has stated that it is unclear from the claim whether Applicants mean to claim a manual method or whether a computer generated program is required.

Claim 17 has been amended accordingly. The term "throwing dice and/or performing drawings" have been deleted. The term "random check generators" has been amended to specify "numerical random check generators". The numerical random check generators are specified as computer programs in claim 4.

Furthermore, the Patent Examiner has stated that it is unclear how one would go about physically making a catalyst form a stochastic method.

Claim 17 has been amended to be drawn at a method for selecting components instead of a method for preparing catalysts. It is well known in the art of computational optimization how to apply numerical random number generators to randomly select items out of a list of items.

It is respectfully requested that the claim rejections regarding the enablement requirement related to the term "Random check generators, throwing dice and/or performing drawings" be withdrawn.

Claim Analysis

The Patent Examiner on page 8 and 9 of the Office Action has required supplying evidence for the statement that it is known in the state of the art to transfer the genetic algorithm from the field of living materials to non living materials.

Applicant submits along with this response an IDS including documents transferring the genetic algorithm from the field of living materials to non living materials.

McLeod et al. describe a genetic algorithm application for the optimization of the distribution of adsorption sites on a two-dimensional catalyst surface. *Sheridan* and *Kearsley* disclosing using a genetic algorithm to suggest combinatorial libraries. *Ugi et al.* as previously submitted discuss heuristic procedures, in particular genetic algorithms, which have been used increasingly in recent years in synthesis planning, chemometrics and combinatorial chemistry *(Ugi, et al., abstract)*.

In addition, we introduced the seminal books *"Adaptation in Natural and Artificial Systems: An Introductory Analysis with Applications to Biology, Control, and Artificial Intelligence" by John H. Holland (MIT Press, 1975)*, and *"Genetic Algorithms in Search, Optimization, and Machine Learning" by David E. Goldberg (AddisonWesley, 1989)*. *Holland* and *Goldberg* discuss a number of different applications of Genetic Algorithms to the field of non-living materials.

However, while genetic algorithms and their terms are generally transferable to abstract optimization problems, it is important to notice that there is no single standard method by which a genetic algorithm generates a new population from the previous one. Methods are usually problem-specific as discussed previously.

The present application specifies a genetic algorithm for selecting components for the preparation of solid catalysts. Claim 17 discloses the following set of method steps:

- the selection according to steps (c), (f) and (i);
- the crossing and mutation of the components in steps (d), (g) and (j);
- the determination of the fitness function for the optimization in steps (e), (h)

and (k).

Applicant believes that claim 17 does convey actual steps and that the method steps are very elaborately disclosed in the present application.

In addition, the Patent Examiner pointed out that the claims as written do not claim "bit strings" of the response of 7/26/2004 and do not refer to an algorithm, therefore the terminology is improper for one of ordinary skill in the art when referring to a catalyst composition or method of making or using a catalyst.

Claim 17 has been amended to be drawn at a method of selecting components of a catalyst. As discussed above, the method steps are elaborately disclosed in the present application. The term "bit strings" has been mentioned in the response of 7/26/2004 while referring to *EP 589,384* cited in the IDS filed February 28, 2001, and not referring to the present application. The specific embodiment of the method in *EP 589,384* relates to bit strings. However, *EP 589,384* has been introduced as one example of a Genetic Algorithm application to a field of non-living materials. There are more applications as discussed above, each being embodied in a problem specific way. It has been

pointed out in the above mentioned response that even if a person skilled in the art were to have attempted to utilize the method disclosed in *EP 589,384* to solid catalysts, he would not have achieved the method specified in Claim 17.

Claim Rejections - 35 USC § 102 / Claim Rejections - 35 USC § 103

1. *Petasis (US 6602817 B1)*

The Patent Examiner on page 11 of the Office Action has rejected Claims 17 and 3 to 15 under 35 U.S.C 102(e) as being anticipated by or in the alternative under 35 U.S.C. 103(a) as being unpatentable over *Petasis (US 6602817 B1)*.

The method of *Petatsis* is related to the background art as disclosed on page 2 and 3 of the specification of the present application. *Petasis* discloses the use of a combination approach to the rapid construction of combinatorial libraries of chiral catalysts, i.e. the construction of a huge list of possible catalysts by a brute force combinatorial combination of possible elements. In a last step, these libraries can then be used to identify the most suitable catalysts for a particular asymmetric transformation.

However, *Petasis* does nowhere disclose a directed optimization of chiral catalysts nor does he suggest the use of an optimization scheme. As discussed on page 3, lines 33-37 of the present application, such a combinatorial approach requires disadvantageously very many syntheses of possible target materials which are timeconsuming and material-intensive.

Claims 17 and 3-15 are therefore not anticipated by or being unpatentable over *Petasis*. It is respectfully requested that the claim rejections over *Petasis* be withdrawn.

2. Kieken, et al. (US 6763309 B2)

The Patent Examiner on page 12 of the Office Action has rejected Claims 17 and 3 to 15 under 35 U.S.C 102(e) as being anticipated by *Kieken, et al. (US 6763309 B2)*.

Kieken, et. al. disclose a method and system for the development of materials. The process relates to a novel decision-support tool (*Kieken, et. al.*, column 6, line 50 onwards). This tool is used interactively in the development of new catalytic materials. Various modeling tools are integrated with a knowledge management system to house the significant experimental and theoretical knowledge for its efficient future

use. The development aims to use the existing knowledge efficiently to develop new catalysts.

However, neither an optimization method nor a Genetic Algorithm is disclosed. A directed optimization following the principles of optimization theory with the particular use of a Genetic Algorithm is not part of knowledge management system as disclosed by *Kieken, et al.*. It is also not suggested.

The Monte Carlo kinetic simulation cited in the Office Action on page 12 is used for the simulation of catalytic properties or performance parameters. In the present application the properties are determined experimentally and not theoretically. A random selection of components as disclosed in the present invention is not part of the invention by *Kieken, et al.*.

Claims17 and 3-15 are therefore not anticipated by *Kieken, et al.*. It is respectfully requested that the claim rejections over *Kieken, et al.* be withdrawn.

3. *Cawse (US 6728541 B1)*

The Patent Examiner on page 13 of the Office Action has rejected Claims 17 and 3 to 15 under 35 U.S.C 102(e) as being

anticipated by *Cawse (US 6728641 B1)*.

Cawse discloses a method and system for selecting a best case set of factors for a chemical reaction. The invention is directed to a method and system for sampling an experimental space for combinatorial high throughput screening (CHTS) (*Cawse*, column 2, lines 19-20). According to the invention, an algorithm can be applied to determine a minimal number of experimental runs necessary to efficiently explore an experimental space by combinatorial high throughput screening. The invention relates to the prior art discussed on page 2 and 3 of the present application. The method is based on n-tuple combinations between so-called identities of a relationship (*Cawse*, abstract).

In contrast, the present invention is not drawn to combinatorial chemistry. The specification discloses a directed optimization employing a Genetic Algorithm. Neither an optimization method nor a Genetic Algorithm application is disclosed or suggested by *Cawse*.

Claims 17 and 3-15 are not anticipated by *Cawse*. It is respectfully requested that the claim rejections over *Cawse* be withdrawn.

4. *Deem, et al. (US 6640191 B1)*

The Patent Examiner on page 13 of the Office Action has rejected Claims 17 and 3 to 15 under 35 U.S.C 102(e) as being anticipated by or in the alternative under 35 U.S.C. 103(a) as being unpatentable over *Deem, et. al. (US 6640191 B1)*.

In conjunction with the present application *Deem, et al.* disclose an optimization process. However, *Deem et al.* disclose a different optimization method, i.e. the use of a Monte Carlo scheme for optimization, not a Genetic Algorithm approach. It is known in the art of optimization theory that the optimization method influences the success of the optimization process greatly.

The process by *Deem, et al.* involves preparing a first set of samples, then changing the composition and non-composition variables of the samples using Monte Carlo sampling methods, and accepting proposed new samples according to a Metropolis acceptance criterion.

In detail, the variables of a randomly chosen sample is changed by a random displacement. The fitness functions or figure of merit of the current sample and its respective newly proposed

sample are directly compared. Proposed samples that increase the figure of merit are always accepted; proposed samples that decrease the figure of merit are accepted with the Metropolis probability (*Deem, et al.*, col. 9, I. 19-21). The optimization scheme involves direct one-to-one comparison of a current and a newly proposed sample out of a list of samples; one is discarded, one is kept.

In contrast, the present invention using a Genetic Algorithm approach compares a set of newly proposed samples to the set of all previously realized samples and from this set the ones having the highest fitness functions are being selected and used for proposing new samples. The old information is not discarded leading to a usually faster and more intelligent optimization scheme compared to Monte Carlo methods. In detail, the Monte Carlo method uses different probabilities (*Deem, et al.* equation (1) and (2), col. 9) compared to the Genetic Algorithm application as discloses (present application, Claim 17 (d), (g) and (j)).

Claims 17 and 3-15 are therefore not anticipated by or as being unpatentable over *Deem, et al.*. It is respectfully requested that the claim rejections over Deem, et. al. be withdrawn.

5. *Schultz, et al. (US Patent No. 6,420,179 B1)*

The Patent Examiner on page 14 of the Office Action has rejected Claims 17 and 3 to 15 under 35 U.S.C 102(e) as being anticipated by *Schultz, et. al. (US Patent No. 6420179 B1)*.

Schultz, et al. disclose a combinatorial synthesis of organometallic materials. It provides methods for parallel synthesis and analysis of novel materials having useful properties. The method of synthesis does not involve an optimization procedure in general, nor a Genetic Algorithm approach in particular.

Claims 17 and 3-15 are therefore not anticipated by *Schultz, et al.*. It is respectfully requested that the claim rejections over *Schultz, et. al.* be withdrawn.

A further reason for the patentability of the present invention is as follows. The present Patent Application is entitled to the benefit of its German priority date of September 11, 1998.

The *Cawse U.S. Patent* has as its earliest reference date January 21, 2000, which is subsequent to September 11, 1998.

Thus, *Cawse* is not prior art, and should be withdrawn as a reference against the present patent application.

The *Deem U.S. Patent* has at its earliest reference date December 30, 1999, which is subsequent to September 11, 1998. Thus, *Deem* is not prior art, and should be withdrawn as a reference against the present patent application.

The *Petasis U.S. Patent* has as its earliest reference date October 23, 1998, which is subsequent to September 11, 1998. Thus, *Petasis* is not prior art, and should be withdrawn as a reference against the present patent application.

The *Kieken U.S. Patent* has as the earliest reference date February 5, 2002, which is subsequent to September 11, 1998. Thus, *Kieken* is not prior art, and should be withdrawn as a reference against the present patent application.

Double Patenting

The Patent Examiner on page 15 of the Office Action has provisionally rejected Claims 17 and 3-15 under the judicially created doctrine of obviousness-type double patenting as being unpatentable over claims 1-9 of copending *Application*

No. 09/909038.

Copending Application has been submitted by the inventors of the present application. It also discloses the use of Genetic Algorithm approach to selection of components of catalysts. However, the form of the optimization step is different. The object of the copending Application is to further improve upon the evolutionary selection strategy and to include catalysts components and performance parameters. The object is achieved by keeping the range of available catalysts in the selection step broader, i.e. some of the original components are not lost after one or a few successive generations. Also, pseudo-components like temperature can be subject to variation.

In this respect it is important to notice that there is no single standard method by which a genetic algorithm generates a new population from the previous one.

Claims 17 and 3-15 are therefore not anticipated by copending *U.S. Patent Application Serial No. 09/909,038.*

To overcome the provisional rejection based on a nonstatutory double patenting ground, the Applicants are filing along with this response, a Terminal Disclaimer in compliance

with 37 CRF 1.321(c). Also enclosed is a check for $65.00 for the U.S.P.T.O. fee. The Commissioner of Patents and Trademarks is hereby authorized to charge any additionally required fee, or to credit any overpayment to our Deposit Account #03-2468.

Respectfully submitted,

DORIT WOLF ET AL

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Enclosures: 1. Second Supplemental IDS
2. Terminal Disclaimer
3. Copy Petition Two Month Extension of Time Small Entity

ERF:lgh

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Maria Guastella